What happens to geometric phase when spin-orbit interactions lift band degeneracy?

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Spin-orbit interaction lifts accidental band degeneracy. The geometric phase $\gamma(C) = \pm\pi$ for circuits surrounding a line of such degeneracy cannot survive completely unchanged. The change depends on how the spin is fixed during adiabatic evolution. For spin fixed along the internal spin-orbit field, $\gamma(C)$ decreases to zero as the circuit collapses around the line of lifted degeneracy. For spin fixed along a perpendicular axis, the conical intersection persists and $\gamma(C) = \pm\pi$ is unchanged.

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Geometric (or Berry) phase[1] has become a powerful tool for analysis of waves in periodic systems, especially electrons in crystals[2,3,4,5,6,7]. Wavevector $\vec{k}$ provides a space in which adiabatic evolution of wavefunctions $\psi_n(\vec{k},\vec{r})$ can be studied. Singular behavior occurs at band degeneracies where energies $\epsilon_1(\vec{k}) = \epsilon_2(\vec{k})$ are equal. In crystals with inversion symmetry, ignoring spin-orbit interactions, degeneracies occur along closed lines in $\vec{k}$-space[8]. The periodic part $u_n(\vec{k},\vec{r}) = \exp(-i\vec{k}\cdot\vec{r})\psi_n(\vec{k},\vec{r})$ of ψ is an eigenstate of $\mathcal{H}(\vec{k}) = (\vec{p}+\hbar\vec{k})^2/2m + V(\vec{r})$. Let the wavevector $\vec{k}(t)$ be given a time evolution which takes it on the circuit C, with $\vec{k}(T) = \vec{k}(0)$. Now suppose that wavefunction evolution is determined by the time-dependent Schrödinger equation with the time-dependent Hamiltonian $\mathcal{H}(\vec{k}(t))$. The time-evolution is assumed adiabatic, namely $u_n(\vec{k},\vec{r},t) \propto u_n(\vec{k}(t),\vec{r})$. Berry's argument shows that $u_n(\vec{k},\vec{r},T)$ differs from $u_n(\vec{k},\vec{r},0)$ by the factor $\exp[i\gamma(C,T)]$, where the phase $\gamma(C,T)$ has two parts, $\gamma(C)+\gamma(T)$. The dynamical part $\gamma(T) = -\int_0^T dt\epsilon_n(\vec{k}(t))/\hbar$ depends on the time elapsed, and the geometric part

$$\gamma(C) = i\oint_C d\vec{k}\cdot\int d\vec{r}u_n^*\vec{\nabla}_k u_n \qquad (1)$$

is invariant and intrinsic to the circuit and the band properties. In particular, $\gamma(C) = \pm\pi$ if C encloses one (or an odd number) of degeneracy lines. This change of wavefunction sign is familiar from other problems where a circuit of adiabatic evolution surrounds a conical intersection. Direct evaluation of Eq.(1) is problematic. Wavefunctions must be continuous and single-valued.

Although gauge invariance is not evident in Eq.(1), Berry gave also an alternate form, for a 3-dimensional parameter space $\vec{k}$, as the flux through a surface S (bounded by C) of a vector $\vec{V}_n$.

$$\gamma(C) = -\int_S d\vec{S}_{\vec{k}}\cdot\vec{V}_n \qquad (2)$$

$$\vec{V}_n = \mathrm{Im}\sum_m \frac{\langle n|\vec{\nabla}_{\vec{k}}\mathcal{H}|m\rangle\times\langle m|\vec{\nabla}_{\vec{k}}\mathcal{H}|n\rangle}{[\epsilon_m(\vec{k})-\epsilon_n(\vec{k})]^2} \qquad (3)$$

The gauge invariance of this vector is evident. Conditions of continuity and single-valuedness of wavefunctions are no longer required. If the circuit surrounds a singularity described by a 2×2 effective Hamiltonian, then the flux equals half the solid angle $\Omega(C)$ subtended in an appropriate scaled space by the circuit as seen from the point of singularity. The appropriate scaled space is the one in which the 2×2 Hamiltonian for states near the conical intersection has the form $\mathcal{H}_{\rm eff} = \vec{R}\cdot\vec{\sigma}$ in terms of scaled coordinates $\vec{R} = (X,Y,Z)$ and Pauli matrices $\vec{\sigma} = (\sigma_x,\sigma_y,\sigma_z)$. This method will be used twice in this paper. The eigenvalues are $\pm R = \rho_z R$, where the quantum number $\rho_z = \pm 1$ is introduced as a branch index. The geometric phase is then $\gamma(C) = -\rho_z\Omega(C)/2$.

Mikitik and Sharlai[7] provide convincing evidence that the geometric phase $\pm\pi$ is seen experimentally as a shift in the semiclassical quantization condition[9] determining the de Haas-van Alphen oscillations. An extreme experimental case is the shifted quantum Hall oscillations originating from orbits near the "Dirac points" in graphene[11,12]. The shifts of quantization condition occur for electron orbits (in a $\vec{B}$-field) which surround a degeneracy line (or point, for graphene.) They also argue[10] that spin-orbit effects can mostly be ignored. This is correct for lighter elements with spin-orbit strength $\xi/\Delta \ll 1$, Δ being any other relevant electron scale such as a band gap. However, the mathematics and the corrections need elucidation. Spin-orbit coupling destroys band degeneracy lines. It is not evident what happens to the geometric phase of $\pm\pi$.

To see the effect of spin-orbit interactions, add to $\mathcal{H}(\vec{k})$ the piece $\mathcal{H}_{SO} = (\vec{\sigma}/4m^2c^2)\cdot\vec{\nabla}V\times(\vec{p}+\hbar\vec{k})$. Choose some point $\vec{k}^*$ of accidental degeneracy, and find energies and eigenstates at nearby $\vec{k}$-points using degenerate $\vec{k}\cdot\vec{p}$ perturbation theory. For notational simplicity, $\vec{k}^*$ is the temporary origin of $\vec{k}$. The degenerate basis functions $|1\rangle$ and $|2\rangle$ are the periodic parts u_1 and u_2 at $\vec{k} = \vec{k}^*$. A phase convention is needed; the coefficients C_G of the expansion $u(\vec{r}) = \sum C_G\exp(i\vec{G}\cdot\vec{r})$ are chosen real. This requires inversion symmetry, which is hereafter assumed. Each state has two spin orientations, so

the effective Hamiltonian matrix is 4×4, with the form

$$\mathcal{H}_{\rm eff} = \begin{pmatrix} \hbar\vec{k}\cdot\vec{v}_a\hat{1} & \hbar\vec{k}\cdot\vec{v}_b\hat{1} - i\vec{\xi}\cdot\vec{\sigma} \\ \hbar\vec{k}\cdot\vec{v}_b\hat{1} + i\vec{\xi}\cdot\vec{\sigma} & -\hbar\vec{k}\cdot\vec{v}_a\hat{1} \end{pmatrix} \qquad (4)$$

where $\hat{1}$ and $\vec{\sigma}$ are 2×2 matrices in spin space. Terms proportional to the 4×4 unit matrix do not mix or split the states and are omitted. The vector $\vec{v}_a$ is $(\vec{v}_1 - \vec{v}_2)/2$, where $\vec{v}_n$ is the band velocity $\vec{\nabla}_k\epsilon_n/\hbar$ at the degeneracy $\vec{k}^*$. The vector $\vec{v}_b$ is the off-diagonal term $\langle 2|\vec{p}/m|1\rangle$, which is pure real since C_G is real. The vector $i\vec{\xi}$ is $\langle 2|\vec{\nabla}V \times \vec{p}|1\rangle/4m^2c^2$. This is pure imaginary since there is also time-reversal symmetry, under an assumption of no magnetic order or external $\vec{B}$-field. Thus three real vectors, $\vec{v}_a$, $\vec{v}_b$, and $\vec{\xi}$, determine the bands near $\vec{k}^*$. The vector $\vec{\xi}$ is a close analog to angular momentum. Consider a system with two degenerate p-states $|x\rangle$ and $|y\rangle$. The angular momentum operator $\vec{L}$ has an imaginary off-diagonal element. The mixed states $|x\rangle \pm i|y\rangle$ are eigenstates of $\vec{L}$ with $\langle\vec{L}\rangle = \pm m\hbar\hat{z}$. The magnitude m deviates from 1 if the point symmetry is less than spherical. The vector $\vec{\xi}$ will be called the "orbit moment."

First suppose that $\vec{\xi} = 0$. Since $\vec{v}_a$ and $\vec{v}_b$ are not generally co-linear, they define a direction of $\vec{k}$, namely $\vec{v}_a \times \vec{v}_b$, along which $\mathcal{H}_{\rm eff} = 0$. This is the direction of the line of degeneracy. After allowing $\vec{\xi} \neq 0$, eigenvalues of Eq.(4) are $\pm\lambda$ where

$$\lambda = \sqrt{\kappa_a^2 + \kappa_b^2 + \xi^2} \qquad (5)$$

with $\kappa_a = \hbar\vec{k}\cdot\vec{v}_a$, $\kappa_b = \hbar\vec{k}\cdot\vec{v}_b$, and $\xi = |\vec{\xi}|$. Each eigenvalue belongs to a Kramers doublet of two opposite spin states. The original degeneracy (without spin-orbit interaction) of 2 (neglecting spin) or 4 (including spin) is lifted everywhere unless $\vec{\xi} = 0$. This should happen only at isolated points in the Brillouin zone, not coinciding with degeneracy lines $\vec{k}^*$. No accidental degeneracies remain, but Kramers degeneracy occurs everywhere. Bands near $\vec{k}^*$ are shown in Fig.1.

The geometric phase under consideration involves a circuit $C(\vec{k})$ surrounding the $\vec{k}^*$ line. A circular path in two-dimensional (κ_a, κ_b)-space, namely $C = (\kappa\cos\phi, \kappa\sin\phi)$, $0 \to \phi \to 2\pi$ is the simplest realization. To calculate $\gamma(C)$, separate Eq.(4) into two similar 2×2 submatrices by choosing basis states with spins polarized along $\vec{\xi}$, which will be used as the z-axis of spin space. The submatrices are

$$\mathcal{H}^{\pm}_{\rm eff} = \begin{pmatrix} \kappa_a & \kappa_b \mp i\xi \\ \kappa_b \pm i\xi & -\kappa_a \end{pmatrix}, \qquad (6)$$

where the upper sign goes with spin up, $\sigma_z = 1$.

The circuit can now be considered as a path $C(\vec{\lambda})$ in a 3-d $\vec{\lambda}$-space, where $(\lambda_x, \lambda_y, \lambda_z) = (\kappa_b, \sigma_z\xi, \kappa_a)$. On this circuit, λ, κ, and ξ are all constant. The effective Hamiltonian has the desired scaled form. The solid angle is $\sigma_z 2\pi(1 - \xi/\lambda)$, so the geometric phase is

$$\gamma(C) = -(\Lambda_z\sigma_z)\pi(1 - \xi/\lambda). \qquad (7)$$

where $\Lambda_z = \pm 1$ is the branch index. This is one of the two main results of this paper. It shows how spin-orbit splitting destroys the simple phase of $\pm\pi$ when the circuit has such a small radius that $\xi \sim \lambda$. If spin-orbit interaction is weak, it does not need a large orbit to have $\xi/\lambda \ll 1$ and approach the full simple phase of $\pm\pi$.

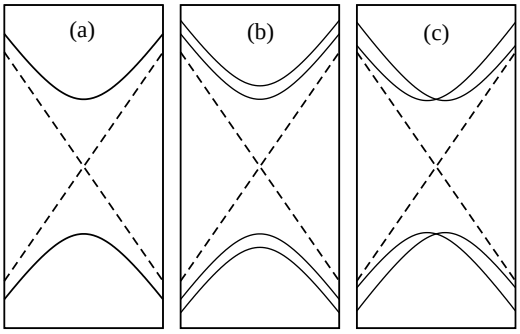

FIG. 1: Energy *versus* $|\vec{k}|$ near the degeneracy point, for (a) no magnetic field, (b) field parallel to $\vec{\xi}$, and (c) field perpendicular to $\vec{\xi}$. The dashed lines are for $\xi = 0$ and $b = 0$; solid lines in panel (a) are $\pm\lambda$, which becomes $\pm\xi$ at the degeneracy point $\vec{k} = 0$.

This is not the full story. The choice to evolve at fixed σ_z was arbitrary. The states of Kramers doublets can be mixed by arbitrary unitary transformations. Evolution of a doublet around a circuit introduces not a simple geometric phase, but a unitary matrix. The $\gamma(C)$ phases just computed are actually the diagonal elements $\exp(\pm i\gamma(C))$ of a 2×2 unitary matrix in the representation with spin quantized along $\vec{\xi}$. It will emerge below that this is indeed the correct adiabatic evolution of the Kramers doublet when an small magnetic field is imposed along the $\vec{\xi}$ direction.

Berry's original argument assumed that $\mathcal{H}$ had a discrete spectrum along C. There is a physically natural way to retain this. Magnetic fields present in experiment since they are used to cause cyclic evolution in $\vec{k}$-space. Magnetic fields also lift Kramers degeneracy. The simplest theoretical device is to add to $\mathcal{H}_{\rm eff}$ a Zeeman term $\mathcal{H}_Z = -\vec{b}\cdot\vec{\sigma}$ coupling only to spin.

To proceed further, an explicit representation of eigenstates is needed. Eigenstates of the effective Hamiltonian (6), labeled by energy $\pm\lambda$ and $\sigma_z = \uparrow, \downarrow$ are chosen as

$$|s\rangle = |-\lambda, \uparrow\rangle = \frac{1}{n}\begin{pmatrix} -\kappa_b + i\xi \\ \kappa_a + \lambda \end{pmatrix} \otimes |\uparrow\rangle, \qquad (8)$$

$$|t\rangle = |-\lambda, \downarrow\rangle = \frac{1}{n}\begin{pmatrix} -\kappa_b - i\xi \\ \kappa_a + \lambda \end{pmatrix} \otimes |\downarrow\rangle, \qquad (9)$$

$$|u\rangle = |+\lambda, \uparrow\rangle = \frac{1}{n}\begin{pmatrix} \kappa_a + \lambda \\ \kappa_b + i\xi \end{pmatrix} \otimes |\uparrow\rangle, \qquad (10)$$

$$|v\rangle = |+\lambda,\downarrow\rangle = \frac{1}{n}\begin{pmatrix}\kappa_a+\lambda\\ \kappa_b - i\xi\end{pmatrix}\otimes|\downarrow\rangle. \qquad (11)$$

These are written as direct product of spatial times spin two-vectors. The normalization is $n=\sqrt{2\lambda(\lambda+\kappa_a)}$. As long as ξ is non-zero, $1/n$ is non-singular and these are smooth, single-valued functions of (κ_a,κ_b), unique except for an arbitrary overall phase, which cannot alter $\gamma(C)$. The lower Kramers doublet $|s\rangle,|t\rangle$ has "orbit moments" $\langle i|\vec{\nabla}V\times\vec{p}/4m^2c^2|i\rangle = \mp(\xi/\lambda)\vec{\xi}$ oriented antiparallel to spin, while the upper Kramers doublet $|u\rangle,|v\rangle$ has identical orbit moments except oriented parallel to spin.

Now the Zeeman term is added. Diamagnetic coupling is neglected. Without loss of generality, the part of the field $\vec{B}=\vec{b}/\mu_B$ perpendicular to ξ can be used to define the x direction of spin. The total Hamiltonian in the basis $|s\rangle,|t\rangle,|u\rangle,|v\rangle$ is

$$\mathcal{H}_{\rm tot} = -\begin{pmatrix} \lambda+b_z & \frac{\kappa}{\lambda}b_x e^{i\omega} & 0 & i\frac{\xi}{\lambda}b_x\\ \frac{\kappa}{\lambda}b_x e^{-i\omega} & \lambda-b_z & -i\frac{\xi}{\lambda}b_x & 0\\ 0 & i\frac{\xi}{\lambda}b_x & -\lambda+b_z & \frac{\kappa}{\lambda}b_x e^{-i\omega}\\ -i\frac{\xi}{\lambda}b_x & 0 & \frac{\kappa}{\lambda}b_x e^{i\omega} & -\lambda-b_z\end{pmatrix} \qquad (12)$$

The factor $(\kappa/\lambda)\exp(i\omega)=\langle s|\sigma_+|t\rangle$ introduces the new angle ω

$$e^{i\omega} = \frac{\lambda}{\kappa} - \frac{\xi(\xi-i\kappa_b)}{\kappa(\lambda+\kappa_a)}. \qquad (13)$$

As the circuit C is followed (ϕ going from 0 to 2π, with ξ,κ,λ constant), ω also evolves from 0 to 2π.

If the field $\vec{b}$ is along z, the upper and lower Kramers doublets are not coupled. The degeneracy is lifted everywhere, and adiabatic evolution proceeds smoothly on the resulting non-degenerate states, yielding the phases $\gamma(C)$ of Eq.(7). The previous discussion was correct. The result 7 can also be obtained directly from Eq.(1) using Eqs.(8,9, 10,11). For fields perpendicular to z, there is both intra- and inter-doublet spin mixing, according to Eq.(12). To first order, since $\vec{b}\ll\lambda$, inter-doublet mixing terms $\pm i\xi b_x/\lambda$ can be neglected, giving 2×2 effective Hamiltonian matrices, of the form

$$\mathcal{H}_{\rm eff}(\vec{b}) = \lambda_z\lambda\hat{1} - \begin{pmatrix} b_z & \frac{\kappa}{\lambda}b_x e^{i\lambda_z\omega}\\ \frac{\kappa}{\lambda}b_x e^{-i\lambda_z\omega} & -b_z\end{pmatrix} \qquad (14)$$

The eigenvalues are

$$\pm\lambda\pm\mu \quad \text{where } \mu^2 = b_z^2 + \frac{\kappa^2}{\lambda^2}b_x^2 \qquad (15)$$

These eigenvalues have an interesting feature: at the degeneracy point $\kappa=0$, in the center of circuit C, $\mu=0$ and Kramers degeneracy is **not** lifted, provided $\vec{b}$ is perpendicular to $\vec{\xi}$. The states at $\vec{k}^*$ have anisotropic g factors which vanish in two directions. The vanishing Zeeman splitting means that a conical intersection, hidden unless $\vec{b}\neq0$, exists exactly where the original band intersection (for $\xi=0$) was located. This also yields a simple geometrical phase of $\pm\pi$. Bands for $\vec{b}\parallel\vec{\xi}$ and $\vec{b}\perp\vec{\xi}$ are shown in Fig.1 panels (b) and (c).

A full calculation of $\gamma(C)$ for the 4 new eigenstates of Eq.(12) is difficult. The Berry method of solid angle works when the basis functions $|1\rangle$, $|2\rangle$ of the 2×2 effective Hamiltonian are fixed at $\vec{k}^*$, whereas the basis functions $|s\rangle,|t\rangle$ or $|u\rangle,|v\rangle$ used in Eq.(14) depend on $\vec{k}$. However, the most important limit remaining to be resolved is when the circuit radius κ is small relative to spin-orbit splitting ξ. In this limit, the basis functions loose their $\vec{k}$-dependence. The relevant scaled parameters are $\vec{\mu}=((\kappa/\lambda)b_x\cos\omega,-\lambda_z(\kappa/\lambda)b_x\sin\omega,b_z)$. The circuit parameterized by ϕ is equally well parameterized by ω which evolves from 0 to 2π. The solid angle in $\vec{\mu}$-space is $2\pi\Lambda_z(1-b_z/\mu)$, so the geometric phase is

$$\gamma(C) = -\pi\beta_z\Lambda_z\left(1-\frac{b_z}{\sqrt{b_z^2+(\kappa/\lambda)^2b_x^2}}\right), \qquad (16)$$

where (Λ_z,β_z) are the two branch indices in the eigenvalue $\pm\lambda\pm\mu=\Lambda_z\lambda+\beta_z\mu$. This is the other main result of this paper. If $b_z=0$, the full geometric phase $\gamma(C)=\pm\pi$ is restored no matter how small the circuit radius. Even though the degeneracy was lifted by spin-orbit interactions, the hidden conical intersection exposed by a Zeeman field controls the result.

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